

Bose-Einstein condensates of polar molecules: anisotropic interactions = anisotropic mass

Andrei Derevianko*

Physics Department, University of Nevada, Reno, Nevada 89557

(Dated: July 22, 2008)

So far the theory of Bose-Einstein condensates (BEC) of polar molecules was based on an ad hoc generalization of equations for spherical atoms. Here I adopt a rigorous pseudo-potential approach to low-energy dipolar interactions and derive a non-linear mean-field Schrödinger equation for a harmonically-trapped condensate. I show that, effectively, the dipolar interactions alter molecular mass. The resulting effective mass is anisotropic: to the leading order the mass is altered only for the motion along the polarizing field. For a typical BEC of spin-polarized magnetically-interacting alkali-metal atoms the effective atomic mass is reduced by 10% from its bare value. For a BEC of polar molecules the mass may be reduced by a factor of a 1,000.

PACS numbers: 03.75.Hh, 34.10.+x

The ongoing quest for a Bose-Einstein condensate of polar molecules[1] is stimulated by a remarkable richness of the quantum phenomena associated with their large dipole-dipole interactions. Inherently anisotropic, the dipolar interactions are crucial to quantum information processing[2] and to realizing exotic states of matter (e.g., topological[3] and checker-board[4] phases) with ultracold molecules.

Background— The intricacies of the many-body problem are rooted in inter-particle interactions that lead to non-separable Hamiltonians. Introducing pseudo-potentials, i.e., effective interactions that are simpler than the original interactions, makes the problem more tractable. In physics of ultracold atoms, all seemingly disparate interactions can be well approximated by a contact pseudo-potential. Its strength is determined by s -wave scattering length a_{ss} , which is computed by solving low-energy scattering problem with the original potential. This contact interaction is central to arriving at the non-linear Schrödinger equation for the condensate wavefunction $\Psi(\mathbf{r})$. The hallmark Gross-Pitaevskii equation [5] (GPE) reads:

$$\left(-\frac{\hbar^2}{2M}\Delta + U(\mathbf{r}) + g'_0 |\Psi(\mathbf{r})|^2\right) \Psi(\mathbf{r}) = \mu_0 \Psi(\mathbf{r}), \quad (1)$$

where μ_0 is the chemical potential, and $U(\mathbf{r})$ is the external confinement potential. The non-linear term arises due to interparticle interactions, $g'_0 = 4\pi\hbar^2/M a_{ss}$. Namely this non-linearity yields a wealth of non-trivial effects, such as solitons, in physics of the condensates [6].

Why do the dipolar interactions require going beyond the conventional approximation? Compared to the $1/r_{12}^6$ dependence of the conventional isotropic van der Waals interactions on interparticle separations, the dipolar interactions are both long-range, $1/r_{12}^3$, and anisotropic.

This seemingly innocuous power-law variation crucially modifies low-energy collision process that underlies the pseudo-potential formalism. Contributions of partial waves beyond the s -wave no longer “freeze out” and the scattering is characterized by an infinite number of scattering lengths. Due to the anisotropy, molecules exert torques on each other and various spherical waves (e.g., s and d) become coupled. These couplings result in additional “anisotropic” scattering lengths [7].

Following Yi and You[8] (YY), the rapidly growing literature on dipolar BECs, see e.g. [8, 9, 10, 11, 12, 13, 14, 15], is based on an effective interaction that is represented as a sum of the contact pseudo-potential and the classical dipole-dipole interaction. This ad hoc approximation has a shortcoming of being valid only in a perturbative (Born) regime. Another, both aesthetic and practical shortcoming, is that in the YY approximation the GPE becomes a non-linear *integro-differential* equation[8] that lacks the appealing minimalism of Eq. (1). By contrast, here, starting from the rigorous quantum-mechanical description of the dipolar collision process [7], we attempt to overcome both shortcomings: (i) the employed pseudo-potential involves scattering parameters that may be tuned all the way through the resonances and (ii) the dipolar GPE derived here has a simple mathematical structure.

Dipolar pseudopotential— In a typical dipolar BEC setup, a molecular gas forms a cloud in an external harmonic trapping potential. Orientation of molecular dipoles D is fixed by applying a polarizing E-field (otherwise, molecular rotations would average dipole moments to zero). Then as $r_{12} \rightarrow \infty$, the molecular interactions acquire dipolar character,

$$V(\mathbf{r}_{12}) \rightarrow \frac{D^2}{|r_{12}|^3} (3 \cos^2 \theta_{12} - 1). \quad (2)$$

Here θ_{12} is the angle between collision axis \mathbf{r}_{12} and the polarizing field. The collision process is also determined by the short-range part of the potential: as molecules approach each other, the electronic clouds start to overlap,

*Electronic address: andrei@AT.unr.edu;
URL: <http://wolfweb.unr.edu/homepage/andrei/tap.html>

and the interactions substantially depart from the dipolar form (2). The YY approximation treats the short- and long-range parts of the full interaction on separate footings; we will incorporate both consistently.

We need to describe a quantum dipolar collision process at ultralow temperatures. I assume that the polarized atoms or molecules follow a unique potential surface. For example, recently attained BEC of highly-magnetic chromium is comprised of spin-polarized atoms [16]. The atoms are trapped in the lowest-energy Zeeman sublevel; transitions to the upper-energy levels are forbidden energetically. To quantify the scattering, one has to solve a multi-channel problem. The relevant scattering parameters are the following limits of the K-matrix characterizing couplings between ℓ and ℓ' partial waves [7],

$$a_{\ell m; \ell' m'} = - \lim_{k \rightarrow 0} \mathcal{K}_{\ell m \rightarrow \ell' m'} / k, \quad (3)$$

where $\hbar k$ is the relative momentum of the colliding pair. K-matrix essentially governs the asymptotic form of the scattering wavefunction for large interparticle separations. Long-range, $1/r_{12}^3$, character of the dipolar interaction ensures that the above limits are finite. The quantities $a_{\ell m; \ell' m'}$ have a dimension of length and will be referred to as scattering lengths.

For illustration, consider scattering lengths for a pure dipolar interaction (i.e., assuming the validity of Eq. (2) for all r_{12}) in the Born approximation. The formalism is described in Ref. [7] and it is based on a system of coupled radial equations for individual partial waves. We find that in the Born approximation both the diagonal and off-diagonal scattering lengths fall off as ℓ^{-2} with increasing ℓ . In the following I assume that the dominant effects are due to $s-s$ and $s-d$ scattering lengths, a_{ss} and a_{sd} . The former is mainly determined by the short-range part of the potential and to the latter by the dipolar coupling. In the Born approximation [7]

$$a_{sd}^{\text{Born}} = -1/(6\sqrt{5}) MD^2/\hbar^2. \quad (4)$$

Values of a_{sd}^{Born} for molecules of present experimental interest are listed in Table I. The off-diagonal scattering length is strongly suppressed (by $\sim (1/137)^2$) for magnetically-interacting atoms: it is -0.01 nm for Cs and -0.2 nm for Cr [16].

	D , Debye	a_{sd}^{Born} , nm
OH ($X^2\Pi_{3/2}$)	1.65	-52
RbCs ($X^1\Sigma$)	1.2	-350
KRb ($X^1\Sigma$)	0.59	-48
NH ($X^3\Sigma^-$)	1.38	-32

TABLE I: Anisotropic scattering length a_{sd} in the Born approximation for molecules of current experimental interest[1].

Pseudopotential — The low-energy pseudopotential for anisotropic scattering was introduced in Ref. [7]. An earlier variational BEC study with this pseudopotential (albeit its erroneous version) was carried out in Ref. [17].

Recently, there was a study of the validity of the pseudopotential approach [18]. These authors found that the pseudopotential description remains accurate as long as a_{sd} is smaller than the characteristic length of the trapping potential.

For the goals of this paper we simplify the rigorous pseudopotential [7]. More details of the discussion presented below can be found in Ref. [19]. We assume that the global BEC properties can be described by well-behaved wavefunctions. In this case we may operate in terms of the momentum-space representation. The matrix element of the pseudopotential between two plane waves $\langle \mathbf{r} | \mathbf{k} \rangle = (2\pi)^{-3/2} e^{i\mathbf{k} \cdot \mathbf{r}}$ is given by $\bar{v}(\mathbf{k}, \mathbf{k}')$ of Ref. [7]. For our case of the dipolar interactions truncated at $s-s$ and $s-d$ couplings it reads $\bar{v}(\mathbf{k}, \mathbf{k}') = \frac{1}{2\pi^2} \frac{\hbar^2}{M} (a_{ss} - a_{sd} \mathcal{F}(\mathbf{k}, \mathbf{k}'))$ with

$$\mathcal{F}(\mathbf{k}, \mathbf{k}') = \sqrt{5} \left\{ P_2(\cos \theta_k) + (k/k')^2 P_2(\cos \theta_{k'}) \right\},$$

where θ_k and $\theta_{k'}$ are angles between the polarizing field and \mathbf{k} and \mathbf{k}' .

Now, under simplifying assumption of harmonic trapping, I transform the momentum-space expression back into the coordinate space. We write for a matrix element of the pseudopotential (cf. Ref. [20] for Rydberg atoms)

$$\langle \psi | \hat{V}_{\text{ps}} | \psi \rangle = (2\pi)^{-3} \int d\mathbf{k} d\mathbf{k}' d\mathbf{r} d\mathbf{r}' \times \\ \psi^*(\mathbf{r}') e^{i\mathbf{k}' \cdot \mathbf{r}'} \bar{v}(\mathbf{k}', \mathbf{k}) \psi(\mathbf{r}) e^{-i\mathbf{k} \cdot \mathbf{r}}. \quad (5)$$

Only certain values of $|\mathbf{k}|$ and $|\mathbf{k}'|$ contribute to this integral. Experimentally, the collisions occur in the presence of harmonic trapping potential, $U(\mathbf{r}) = \frac{1}{2} M (\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2)$. For two harmonically-confined particles the center-of-mass and relative motions decouple and the Hamiltonian for the relative motion reads $H_r = p_{12}^2/(2\mu) + (\frac{\mu}{M}) U(|\mathbf{r}_{12}|) + V(\mathbf{r}_{12})$, where $V(\mathbf{r}_{12})$ is the full interaction potential between the particles and $\mu = M/2$. In the stationary problem we solve the eigenvalue equation $H_r \psi(\mathbf{r}_{12}) = E_r \psi(\mathbf{r}_{12})$, E_r being the energy of the relative motion. Ref. [21] presented a numerical comparison of solutions of this equation with the full molecular potential and its pseudopotential representation (for isotropic s -wave scattering). They observed that for velocity-dependent potentials the relevant collision momentum k_c is $\hbar^2 k_c^2/(2\mu) = E_r$. Indeed, the collision process occurs at $|\mathbf{r}_{12}|$ much smaller than the harmonic length. In this region $U(|\mathbf{r}_{12}|) \approx 0$ and the kinetic energy is E_r . This leads to $k_c^2 = 3/2 M \bar{\omega}/\hbar$, with $\bar{\omega} = \sum_i \omega_i/3$ being the average of the three trapping frequencies.

Returning to the evaluation of the integral (5), we see that the relevant contributions are accumulated at $|\mathbf{k}| = |\mathbf{k}'| = k_c$. Representing $\cos \theta_k = k_z/k$, and using the

properties of the Dirac δ -function, we arrive at

$$\hat{V}_{\text{ps}}(\mathbf{r}_{12}) \approx 4\pi \frac{\hbar^2}{M} \delta(\mathbf{r}_{12}) \times \left\{ a_{ss} + \sqrt{5} a_{sd} \left[1 + \frac{3}{2} \frac{1}{k_c^2} \left(\overleftarrow{\partial}_{z_{12}}^2 + \overrightarrow{\partial}_{z_{12}}^2 \right) \right] \right\}. \quad (6)$$

This is a contact interaction that depends on the traditional s -wave scattering length a_{ss} and “anisotropic” scattering length a_{sd} . The latter is due to the dipolar coupling of s and d partial waves. Both scattering lengths are to be determined from multi-channel scattering calculations with the full interaction potential. One recognizes the conventional contact interaction $4\pi\hbar^2/M \delta(\mathbf{r}_{12}) a_{ss}$ for the s -wave scattering; the remaining part, with a_{sd} , is due to the dipolar interactions. In this term the $\overleftarrow{\partial}_{z_{12}}^2 \equiv \partial^2/\partial z_{12}^2$ acts on the bra and $\overrightarrow{\partial}_{z_{12}}^2$ operates on the ket. The dipolar contribution to \hat{V}_{ps} breaks into two parts: isotropic and anisotropic (derivative) terms. The isotropic dipolar contribution merely renormalizes the traditional spherically-symmetric pseudopotential. It is the derivative term that defines the novel physics of the dipolar BEC. The anisotropy is imposed by the polarizing field (the derivatives are taken along the field). The long-range character of the dipolar interactions is manifested through k_c^2 which characterizes the entire trapping potential.

The low-energy dipolar interactions can be controlled by external fields. As in the case of Feshbach-resonance tunability of a_{ss} , the anisotropic length a_{sd} may exhibit resonances. There is an evidence for such a field-dependent resonance in dipolar collisions of E-field-polarized Rb atoms [22]. This opens an intriguing possibility of *resonantly* controlling and enhancing dipolar interactions in BECs. The described resonant scattering mechanism is to be distinguished from a recent proposal [23] on controlling the strength of the dipolar interaction by modulating the dipoles by oscillating fields.

Mean-field approximation — With the derived pseudo-potential, I proceed to analyzing properties of the dipolar BEC. In the mean-field approximation, all identical bosons occupy the same single-particle wavefunction $\Psi(r)$. Under this assumption, we arrive at the total energy of the condensate (Ψ is normalized to the total number of particles N)

$$E[\Psi] = \int d\mathbf{r} \left(\frac{\hbar^2}{2M} |\nabla \Psi|^2 + U(\mathbf{r}) |\Psi|^2 + \frac{1}{2} g_0 |\Psi|^4 - g_d \left(\frac{\partial}{\partial z} |\Psi|^2 \right)^2 \right), \quad (7)$$

where the isotropic and anisotropic coupling parameters are defined as

$$g_0 = 4\pi\hbar^2/M \left(a_{ss} + \sqrt{5} a_{sd} \right), \quad (8)$$

$$g_d = 2\pi\hbar^3/(M^2\bar{\omega}) \sqrt{5} a_{sd}. \quad (9)$$

The dipolar effects are governed by the anisotropic length a_{sd} . Dipolar interactions modify the traditional GP term $\frac{1}{2}g_0|\Psi|^4$ and appear in the newly-introduced derivative term, $-g_d(\partial_z|\Psi|^2)^2$.

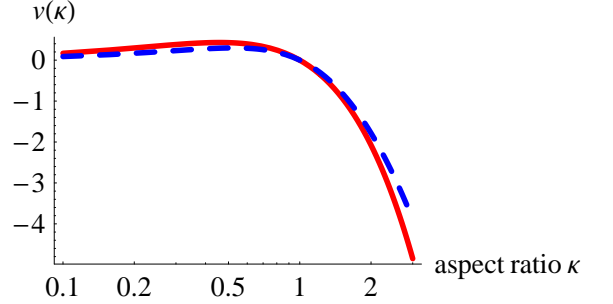


FIG. 1: Comparison of the dipolar interaction energy computed in the traditional YY approximation (solid line) and within the present pseudo-potential approach (dashed line). The comparison is given as a function of the aspect ratio of the cloud.

In the present analysis, we truncated the expansion over partial waves at the $s-s$ and $s-d$ scattering lengths. To estimate the truncation error, we turn to the regime where the Born approximation is valid. Then we use Eq.(4) and compare the results with those computed within the conventional YY approximation. In particular, consider an important expectation value $\langle V_{DD} \rangle$ of the dipolar interaction for an axially-symmetric ground state of the harmonic trapping potential ($\omega_x = \omega_y \equiv \omega_\perp$, aspect ratio $\kappa = (\omega_z/\omega_\perp)^{1/2}$, polarizing field is along the axis of symmetry). We may parameterize $\langle V_{DD} \rangle = N\hbar\omega_\perp (a_{sd}^{\text{Born}}/a_\perp) \times v(\kappa)$. In the YY approximation $v^{YY}(\kappa) = -6\kappa/(\sqrt{2\pi}) b(\kappa)$, where function $b(\kappa)$ is given in Ref. [8]. In the present pseudo-potential approach $v^{ps}(\kappa) = \sqrt{\frac{5}{2\pi}} \left(\kappa - \frac{3\kappa^3}{(\kappa^2+2)} \right)$. A comparison of the two reduced dipolar energies v^{ps} and v^{YY} as functions of the aspect ratio is presented in Fig.1. We find a good agreement between the two curves. Both energies vanish for spherically-symmetric ($\kappa = 1$) traps.

Effective anisotropic mass— For real-valued Ψ , we combine the kinetic-energy and the derivative terms in Eq. (7). The result suggests introducing effective mass along the polarizing field,

$$M_{zz}^{\text{eff}}(\mathbf{r}) = M/(1 - 8g_d M n(\mathbf{r})/\hbar^2), \quad (10)$$

where the number density $n(r) = |\Psi(r)|^2$. The mass remains “bare” (M) for the motion perpendicular to the polarizing field. In the Born approximation, the relative change in the mass is

$$\frac{\delta M_{zz}^{\text{eff}}}{M} \approx -\frac{8\pi}{3} \frac{n(r) D^2}{\hbar\bar{\omega}},$$

i.e., the mass is reduced from its bare value by the ratio of the characteristic dipole interaction $n(r)D^2$ to the trapping energy. As an illustration, consider a BEC of alkali-metal atoms (magnetic moment $1\mu_B$) with $n \approx 10^{14} \text{ 1/cm}^3$ in a trap of $\bar{\omega} = 2\pi \times 100 \text{ Hz}$. We find that the mass is reduced by 10%. For a BEC of molecules the effect is even more pronounced. Here the effective mass is about a 1,000 times smaller than the bare mass.

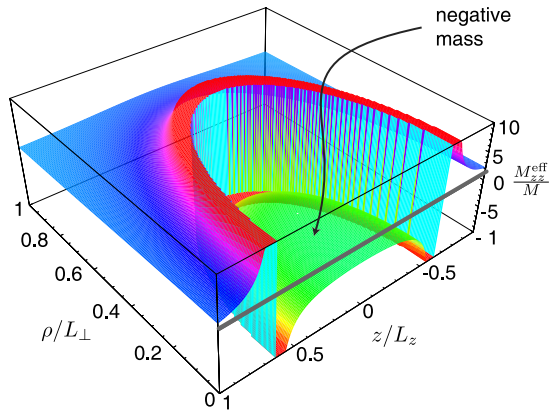


FIG. 2: Effective anisotropic mass $M_{zz}^{\text{eff}}(\mathbf{r})$ as a function of position for an “anomalous” ($a_{sd} > 0$) BEC in a harmonic trapping potential. An unperturbed Gaussian density profile of cylindrical symmetry about the polarizing field is assumed, $n(\mathbf{r}) = n_{\text{max}} \exp\{-(\rho/L_{\perp})^2 - (z/L_z)^2\}$. The peak density is chosen to exceed the critical value, $n_{\text{max}} > \hbar^2/(8Mg_d)$, and the effective mass M_{zz}^{eff} is negative in the center of the cloud. As we move to the outer regions of the cloud, n decreases, M_{zz}^{eff} goes through a singularity and becomes positive. For even smaller densities, M_{zz}^{eff} approaches the bare mass M .

The effective mass depends on the local density. Especially interesting is the case when a_{sd} is tuned to positive values: here the effective mass may become *negative* (see Fig. 2). Here the condensate is unstable in the region of negative mass: the energy may be lowered by accumulating density oscillations of increas-

ingly shorter wavelengths. By requiring that at the peak density $M_{zz}^{\text{eff}} > 0$, we find that the BEC is stable for a number of molecules below the critical number $N < N_{\text{crit}} \approx 1/8\sqrt{\pi/5}\sqrt{\hbar/(M\omega_z)}/a_{sd}$. Such an instability is not present in the traditionally-considered dipolar gases, as $a_{sd}^{\text{Born}} < 0$. We observe that the instability in this case is likely to be related to the well-known instability due to attractive isotropic interactions [6] (when the effective scattering length $a_{ss} + \sqrt{5}a_{sd} < 0$).

Finally, we minimize Eq. (7) with respect to Ψ , and arrive at the non-linear Schrödinger equation

$$\left(-\frac{\hbar^2}{2M}\Delta + U(\mathbf{r}) + g_0|\Psi(\mathbf{r})|^2\right)\Psi(\mathbf{r}) + g_d\left(\frac{\partial^2}{\partial z^2}|\Psi(\mathbf{r})|^2\right)\Psi(\mathbf{r}) = \mu_0\Psi(\mathbf{r}). \quad (11)$$

This equation subsumes the traditional GPE (1) when $a_{sd} = 0$, i.e., for bosons interacting via spherically-symmetric forces. Dipolar length a_{sd} modifies the isotropic term and it governs the derivative term. By contrast to the so far employed YY approximation, Eq.(11) is more concise and remains valid even in a vicinity of scattering resonances.

To conclude, here I developed a new framework for analyzing dipolar BECs. The principal results are: the dipolar pseudopotential (6), the energy functional (7), and the mean-field equation (11). The results may be interpreted in terms of the effective anisotropic mass: I showed that the interactions between dipoles alter mass for a motion along the polarizing field. For a typical BEC of spin-polarized magnetically-interacting alkali-metal atoms the effective mass is reduced by 10% from its bare value. For a BEC of polarized heteronuclear molecules the mass may be reduced by a factor of a 1,000.

This work was supported in part by the National Science Foundation and by the National Aeronautics and Space Administration under Grant/Cooperative Agreement No. NNX07AT65A issued by the Nevada NASA EPSCoR program.

-
- [1] Eur. Phys. J. D **31**, 149 (2004), special Issue on Ultracold Polar Molecules: Formation and Collisions.
 - [2] D. DeMille, Phys. Rev. Lett. **88**, 067901 (2002).
 - [3] A. Micheli, G. K. Brennen, and P. Zoller, Nat. Phys. **2**, 341 (2006).
 - [4] K. Góral, L. Santos, and M. Lewenstein, Phys. Rev. Lett. **88**, 170406 (2002).
 - [5] E. P. Gross, Nuovo Cimento **20**, 454 (1961); E. P. Gross, J. Math. Phys. **4**, 195 (1963); L. P. Pitaevskii, Zh. Eksp. Teor. Fiz. **40**, 646 (1961) [Sov. Phys. JETP **13**, 451 (1961)].
 - [6] C. J. Pethick and H. Smith, *Bose-Einstein condensation in dilute gases* (University Press, Cambridge, UK, 2002).
 - [7] A. Derevianko, Phys. Rev. A **67**, 033607 (2003), Phys. Rev. A **72**, 039901(E) (2005).
 - [8] S. Yi and L. You, Phys. Rev. A **63**, 053607/1 (2001).
 - [9] L. Santos, G. V. Shlyapnikov, P. Zoller, and M. Lewenstein, Phys. Rev. Lett. **85**, 1791 (2000).
 - [10] D. H. J. O'Dell, S. Giovanazzi, and C. Eberlein, Phys. Rev. Lett. **92**, 250401 (2004).
 - [11] J. Stuhler, A. Griesmaier, and T. Koch et al., Phys. Rev. Lett. **95**, 150406 (2005).
 - [12] P. Pedri and L. Santos, Phys. Rev. Lett. **95**, 200404 (2005).
 - [13] N. R. Cooper, E. H. Rezayi, and S. H. Simon, Phys. Rev. Lett. **95**, 200402 (2005).
 - [14] S. Ronen, D. C. E. Bortolotti, and J. L. Bohn (2006), cond-mat/0607704.

- [15] Y. Kawaguchi, H. Saito, and M. Ueda, Phys. Rev. Lett. **97**, 130404 (2006).
- [16] A. Griesmaier, J. Werner, S. Hensler, J. Stuhler, and T. Pfau, Phys. Rev. Lett. **94**, 160401 (2005).
- [17] S. Yi and L. You, Phys. Rev. Lett. **92**, 193201 (2004).
- [18] K. Kanjilal, J. L. Bohn, and D. Blume, Phys. Rev. A **75**, 052705 (2007).
- [19] A. Derevianko, *Simplified contact pseudopotential for anisotropic interactions of polarized particles under harmonic confinement* (2008), arXiv.org:0807.3111.
- [20] A. Omont, J. Phys. (France) **38**, 1343 (1977).
- [21] D. Blume and C. H. Greene, Phys. Rev. A **65**, 043613 (2002).
- [22] B. Deb and L. You, Phys. Rev. A **64**, 022717/1 (2001).
- [23] S. Giovanazzi, A. Görlitz, and T. Pfau, Phys. Rev. Lett. **89**, 130401 (2002).